



# wwPDB NMR Structure Validation Summary Report ⓘ

Oct 28, 2024 – 05:09 pm GMT

PDB ID : 1QNZ  
Title : NMR structure of the 0.5b anti-HIV antibody complex with the gp120 V3 peptide  
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

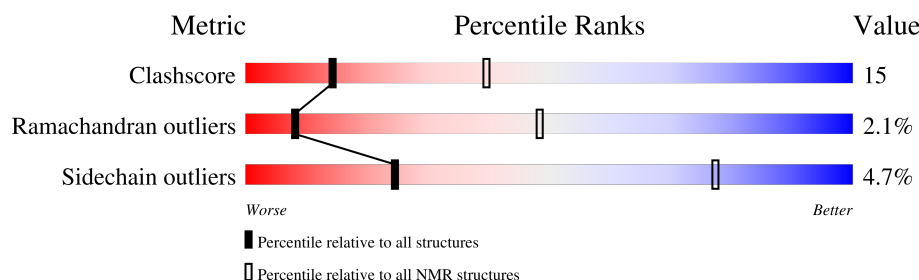
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	H	119	
2	L	112	
3	P	18	

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3813 atoms, of which 1870 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 0.5B ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						Trace
1	H	119	Total	C	H	N	O	S	0
			1826	595	888	151	187	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	137	SER	PHE	conflict	GB 254221

- Molecule 2 is a protein called 0.5B ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms						Trace
2	L	112	Total	C	H	N	O	S	0
			1686	538	823	144	178	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	72	ARG	GLY	conflict	UNP P01665
L	112	ARG	-	expression tag	UNP P01665

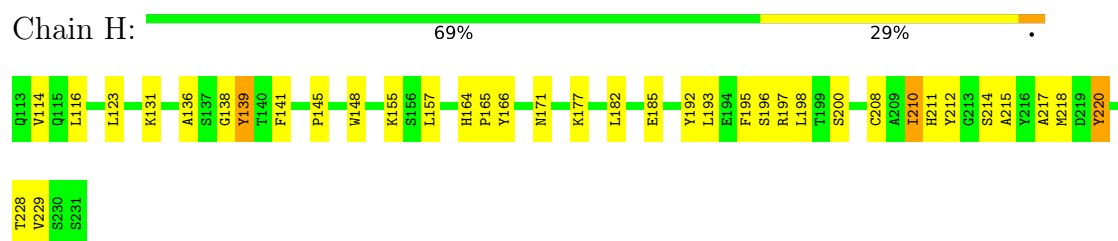
- Molecule 3 is a protein called GP120.

Mol	Chain	Residues	Atoms						Trace
3	P	18	Total	C	H	N	O		0
			301	88	159	32	22		

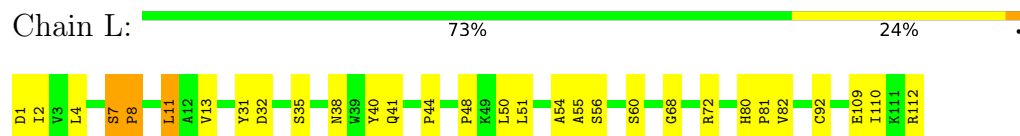
## 4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

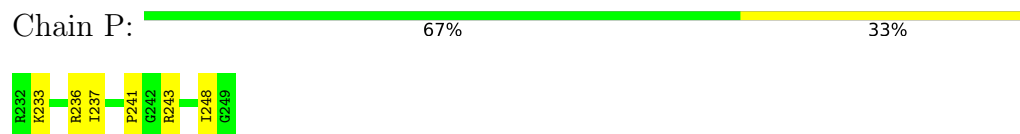
### • Molecule 1: 0.5B ANTIBODY (HEAVY CHAIN)



### • Molecule 2: 0.5B ANTIBODY (LIGHT CHAIN)



### • Molecule 3: GP120



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.8
NMRDraw	structure solution	
NMRView	structure solution	
X-PLOR	structure solution	3.8

No chemical shift data was provided.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	H	938	888	884	34
2	L	863	823	822	26
3	P	142	159	156	6
All	All	1943	1870	1862	58

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

5 of 58 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:H:217:ALA:HB2	2:L:38:ASN:CG	0.78	2.00
1:H:195:PHE:HB3	1:H:198:LEU:HD21	0.77	1.55
1:H:200:SER:HA	1:H:229:VAL:HG11	0.69	1.65
2:L:41:GLN:HB2	2:L:51:LEU:HD11	0.68	1.66
1:H:116:LEU:HD13	1:H:208:CYS:O	0.67	1.89

### 6.3 Torsion angles [i](#)

#### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	117/119 (98%)	101 (86%)	16 (14%)	0 (0%)	100	100
2	L	110/112 (98%)	89 (81%)	16 (15%)	5 (5%)	3	27
3	P	16/18 (89%)	15 (94%)	1 (6%)	0 (0%)	100	100
All	All	243/249 (98%)	205 (84%)	33 (14%)	5 (2%)	8	48

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	L	8	PRO
2	L	32	ASP
2	L	44	PRO
2	L	60	SER
2	L	72	ARG

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	102/102 (100%)	97 (95%)	5 (5%)	23	76
2	L	95/95 (100%)	91 (96%)	4 (4%)	27	80
3	P	14/14 (100%)	13 (93%)	1 (7%)	15	65
All	All	211/211 (100%)	201 (95%)	10 (5%)	24	77

5 of 10 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	H	139	TYR
1	H	155	LYS
1	H	171	ASN
1	H	210	ILE
1	H	220	TYR



### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided